GOZCARDS (Global OZone Chemistry And Related trace gas Data records for the Stratosphere): Progress in merging stratospheric datasets

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Project Overview

- Global (satellite) measurements of the state of stratospheric composition help to
  > understand atmospheric variability and long-term change
  > constrain models that, in turn, may provide better predictions of future change
- While 4 to 5 yrs of data can provide detailed views and "climatology",
  this is not long enough for studying/understanding long-term change.
- GOZCARDS focuses on the long-term satellite data record (from 1979 to the current timeframe of satellite measurements from Aura MLS and ACE-FTS)
  > to compile and characterize the changing stratospheric state (binned time series) for key chemical species: O_3, HCl, ClO, ClOx, HF, H_2O, CH_4, N_2O, NO, NO_2, NOx, HNO_3
  > merging of datasets from different instruments is needed

Motivation (quotes):

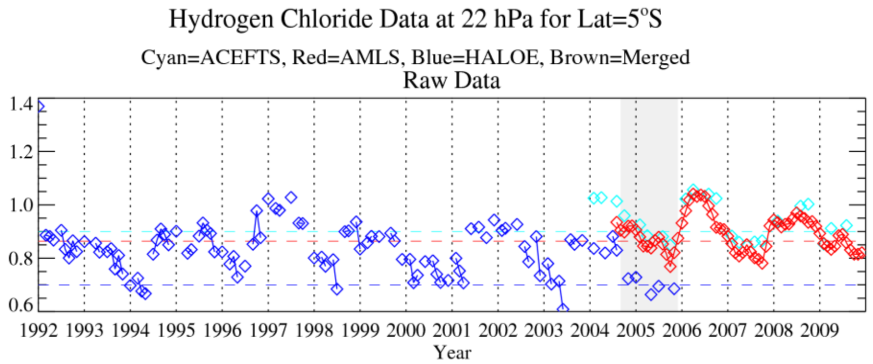
"Data sets encapsulating the behaviour of the Earth system are one of the greatest technological achievements of our age – one of the most deserving of future investment."

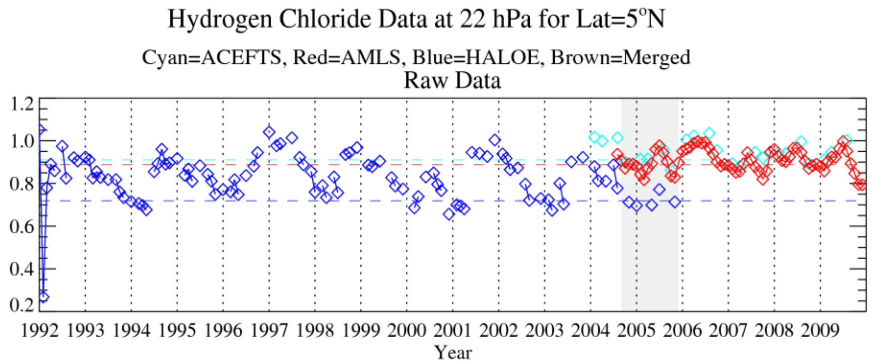
Nature, vol. 450, Dec. 2007, pg. 761, "Patching together a world view."

"Documenting trends and long-term changes is essential for understanding many natural phenomena. Because the state of natural systems is never repeated, data losses, or missed data collection opportunities can never be corrected. Consequently, the value of Earth and space science data grows with time, placing a premium on long-term data curation. Accurate, complete, and, when possible, standardized metadata are as important as the data themselves. Earth and space science data are a world heritage. ***Taking care of such data is our responsibility and our obligation to future generations.****"*

AGU Policy Statement excerpts; statement from May 1997, revised and reaffirmed May 2009.
For full statement, see http://www.agu.org/sci_pol/positions/geodata.shtml

HCl: merging datasets





- **Cases exist (at low latitudes) when no overlap exists between all 3 datasets (HALOE, ACE-FTS, Aura MLS)**
  [no common (colocated) months for comparing all 3 datasets]
  > even with 1.5 yrs of overlap (HALOE & ACE-FTS "skip turns" viewing low lats.)

  → One cannot "directly" calculate an average of the 3 datasets and merge these

- **Instead, we merge "iteratively" by using the dataset with best monthly coverage (MLS), so as to get avg. offsets versus the other ones (separately)**

  > First, merge ACE-FTS (or dataset 1) and Aura MLS; this temporary merge (TM) provides monthly coverage that (now) overlaps with HALOE (or dataset 2)
  > Get average reference from avg. of TM (weighted by 2/3) & HALOE (weighted by 1/3)
  - Get offsets with respect to this avg. reference
  > Final merge of 3 datasets (using offsets vs avg. reference)

Long-term data records: MEaSUREs GOZCARDS products (& investigators)

Stratospheric Products	Planned Satellite Datasets / Main investigators
O_3 (zonal mean time series) See *Wang et al.* poster	SAGE I, SAGE II, SAGE III, HALOE, UARS MLS, ACE-FTS, Aura MLS (+ POAM as a check) [**RW**, JA, LF]
HCl (zonal mean series)	HALOE,ACE-FTS, Aura MLS [**LF**, RF,JA]
ClO (zonal mean series)	UARS & Aura MLS [*Nedoluha et al., JGR*, in review, →no offsets needed between UARS and Aura]
ClO_x (zonal mean series)	UARS MLS, Aura MLS [**RS/TC** + LF, MSa, RF]
HNO_3 (zonal mean series) See *Fiorucci et al.* poster	UARS MLS,ACE-FTS,Aura MLS (Odin/SMR as check) [LF/Msa, Fiorucci/Muscari] study of potential offsets
H_2O (zonal mean series)	SAGE II, HALOE, ACE-FTS, Aura MLS [**JA**, RW, LF, RF] (+ POAM data as a check)
N_2O (zonal mean series)	ACE-FTS, Aura MLS [**LF**]
NO_2 (zonal mean series)	SAGE II, HALOE, POAM III, ACE-FTS [**RW**, JA, LF]
NO (zonal mean series)	HALOE, ACE-FTS [**JA**, LF]
NO_x (zonal mean series)	SAGE II, HALOE, POAM III, ACE-FTS [**RS/TC**, RW, JA, LF]
CH_4 (zonal mean series)	HALOE, ACE-FTS [**JA, LF**]
HF (zonal mean series)	HALOE, ACE-FTS [**JA**, LF, …] → HF still increasing
T (zonal mean series)	GMAO MERRA reanalysis [**MSc**, VP, GM, LF]
EqL/θ binned products	All of the above (lower priority) [LF, RF, GM, MSa, MSc]

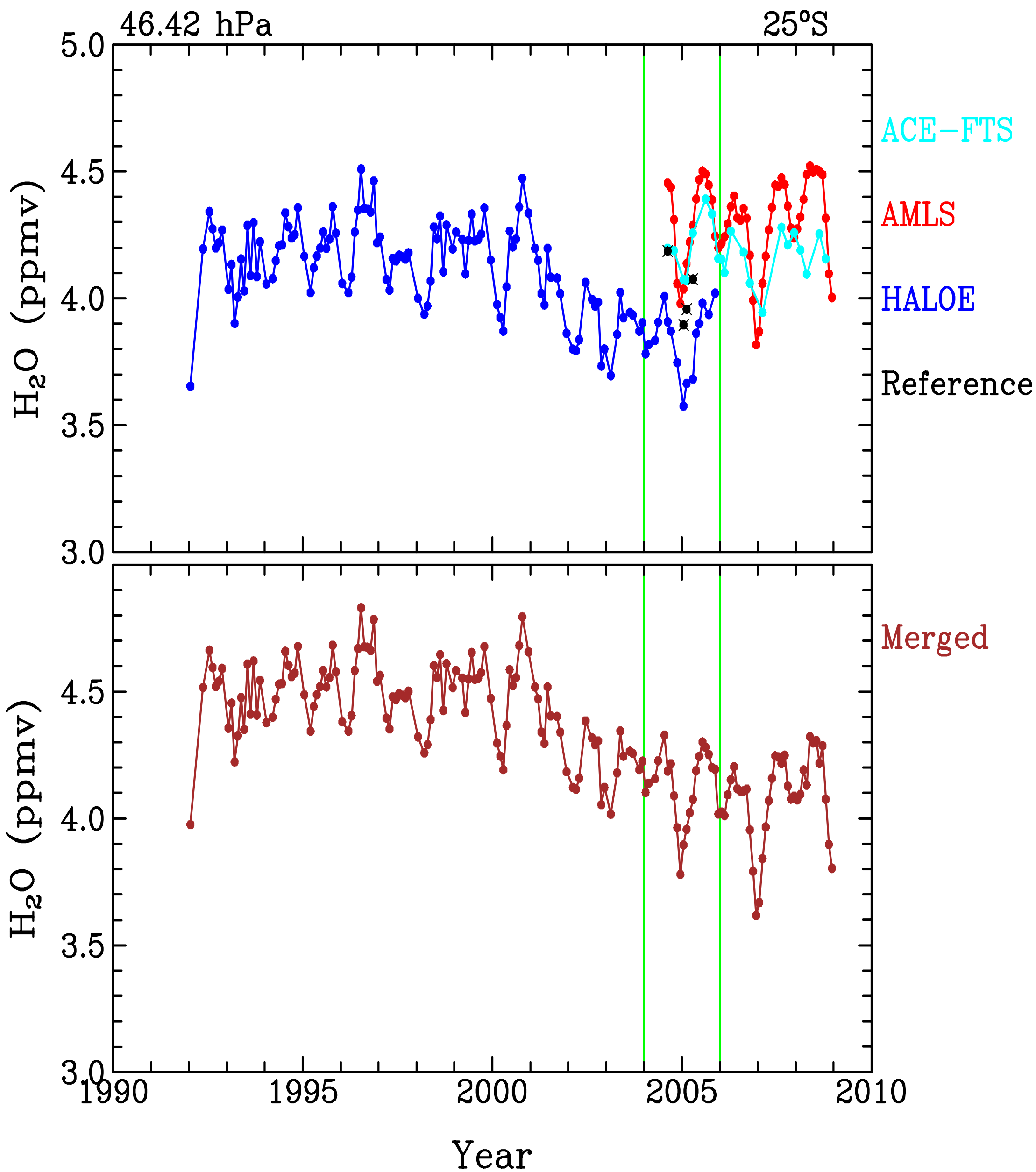
MEaSUREs GOZCARDS Team

Co-investigators
- M. Santee (JPL)
- M. Schwartz (JPL)
- J. Anderson (Hampton Univ.)
- R. Wang (GATech)
- R. Salawitch(UMCP)

Collaborators
- P. Bernath
- K. Walker
- T. Canty
- *D. Cunnold*
- K. Hoppel
- N. Livesey
- G. Manney
- S. Pawson
- J. Russell
- I. Fiorucci, G. Muscari,
- B. Connor,G. Nedoluha

+ others at JPL
(R. Fuller, B. Knosp,…)

H_2O



- **Merging Datasets: Simple case (use H_2O as an example)**

1) Averages of overlapping Aura MLS, ACE-FTS and HALOE datasets are calculated.

2) Constant offsets from each individual dataset are obtained with respect to the reference (here, the average of the overlapping zonal averages).

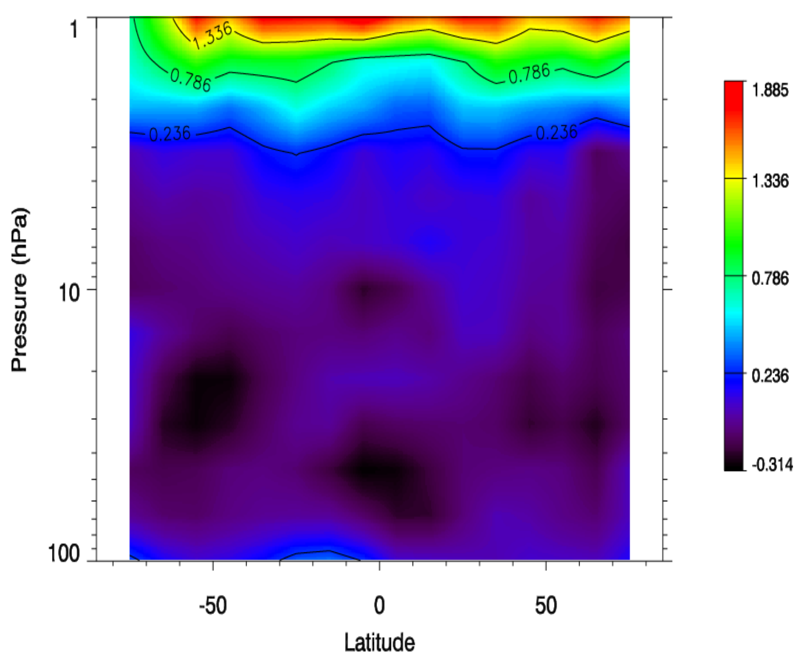
3) Each time-series is then adjusted by the appropriate offset.

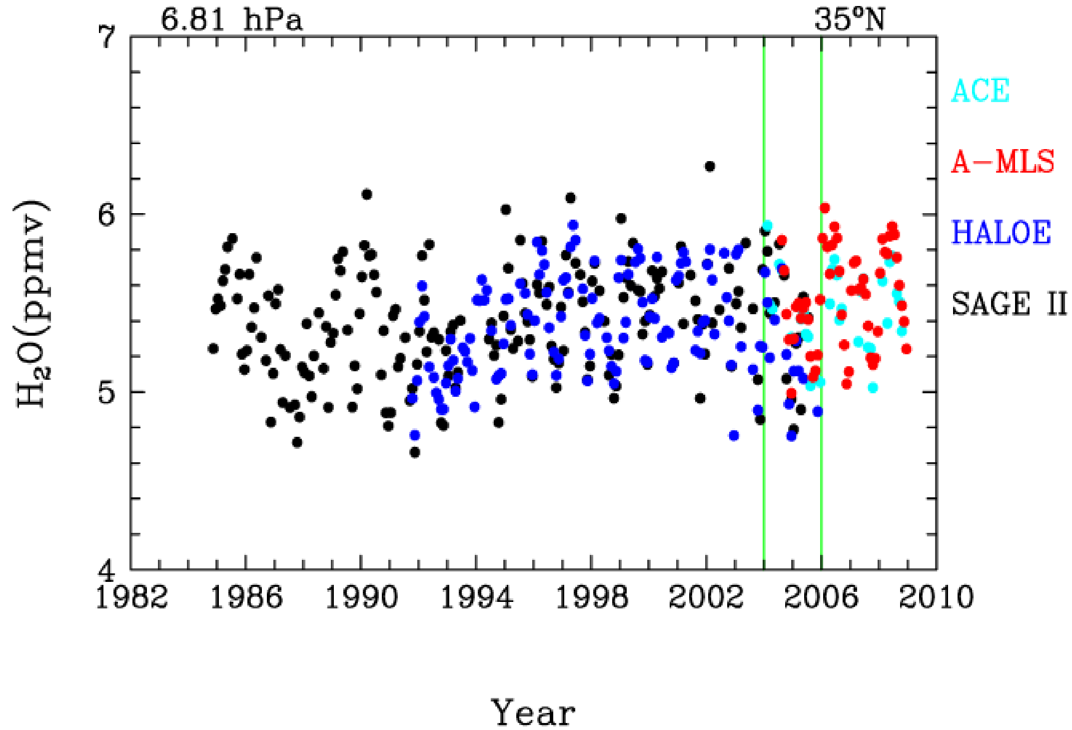
4) A merged time-series is then calculated by averaging the available adjusted data sets.

- **We have been refining / adapting the merging procedure [see HCl examples]**

H_2O

Also adding SAGE II data to enable data record starting in 1984





SAGE II – HALOE

The avg. H_2O differences increase in the upper stratosphere - and SAGE II differs more there versus other datasets as well

→ SAGE II H_2O data will not be included for pressures less than ~ 3 hPa.

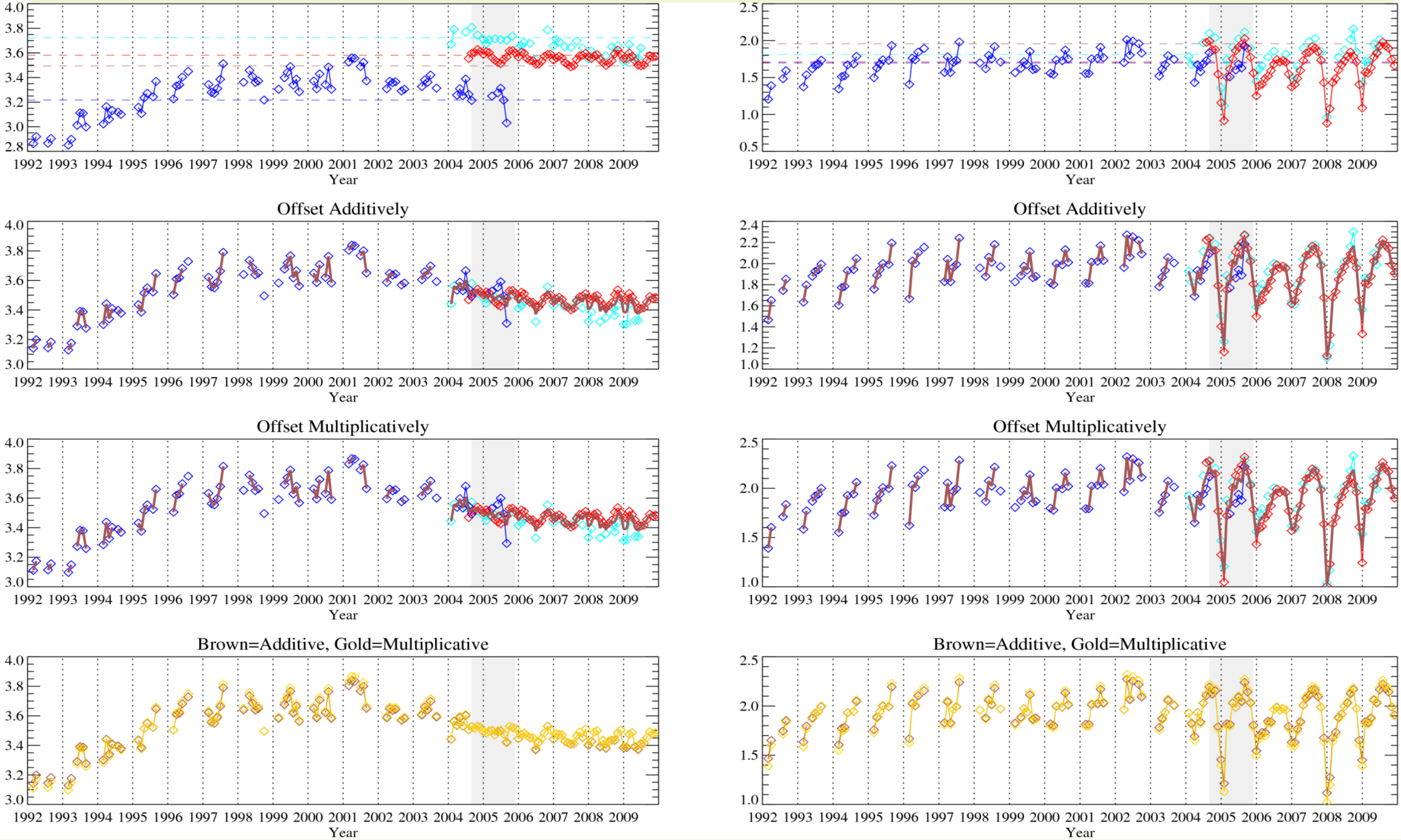
Sample H_2O time series using **SAGE II**, **HALOE**, **ACE-FTS**, and **Aura MLS** data (for 30˚N-40˚N at 7 hPa). The green vertical lines bound the overlap period for all 4 measurements.

SAGE II H_2O data were already calibrated using the HALOE data [calibration issue for SAGE II] (but SAGE II trends should be negligibly affected).

HCl: merging datasets

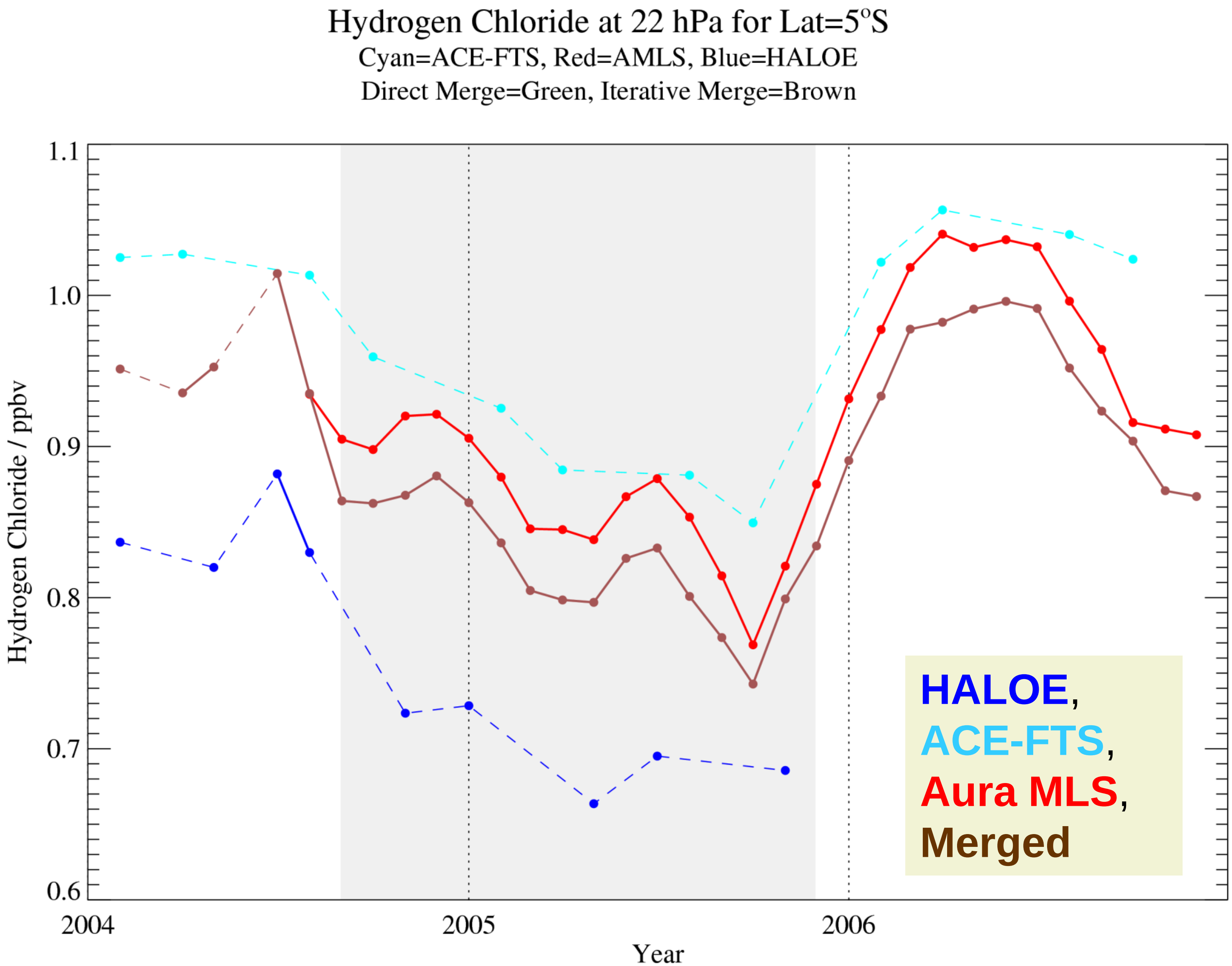
HALOE, ACE-FTS, Aura MLS, Merged

0.5 hPa, 65˚N **32 hPa, 65˚N**



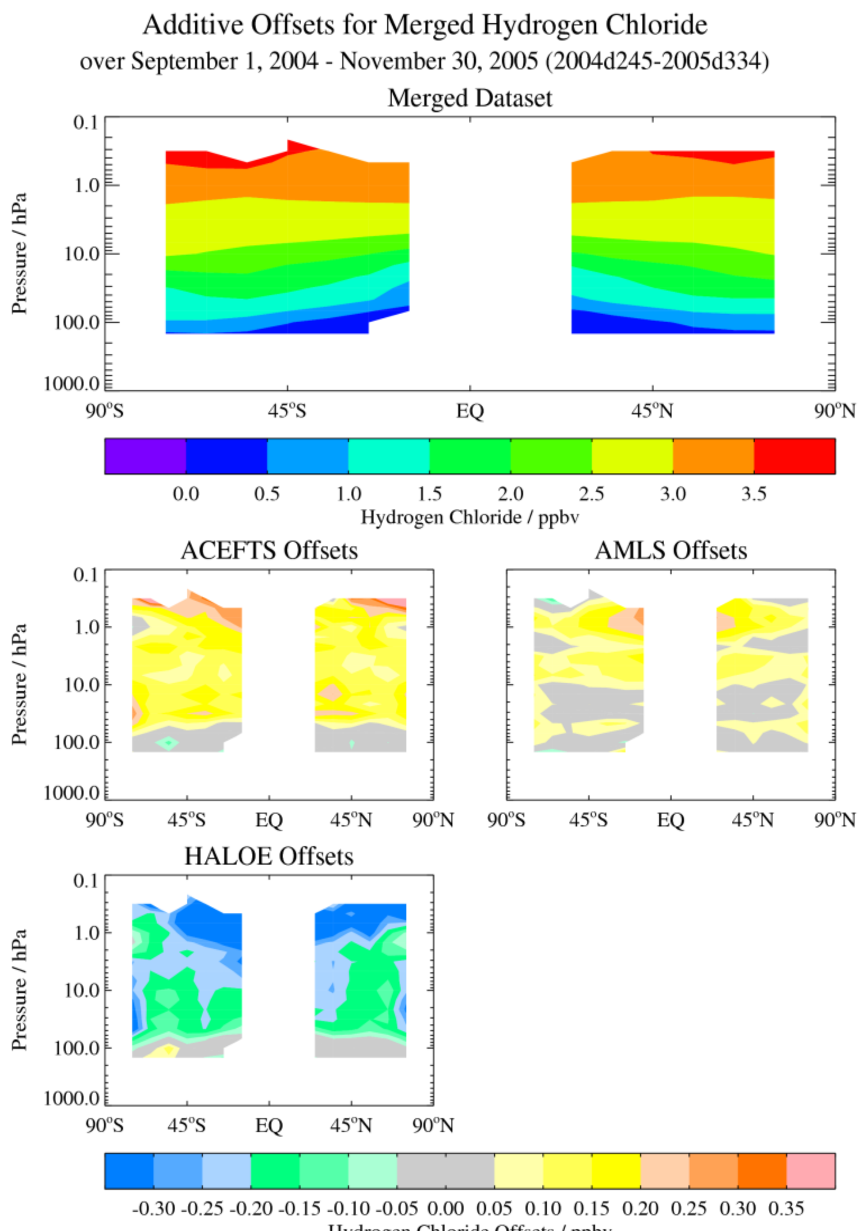
Additive & multiplicative offsets have been investigated (generally small differences)

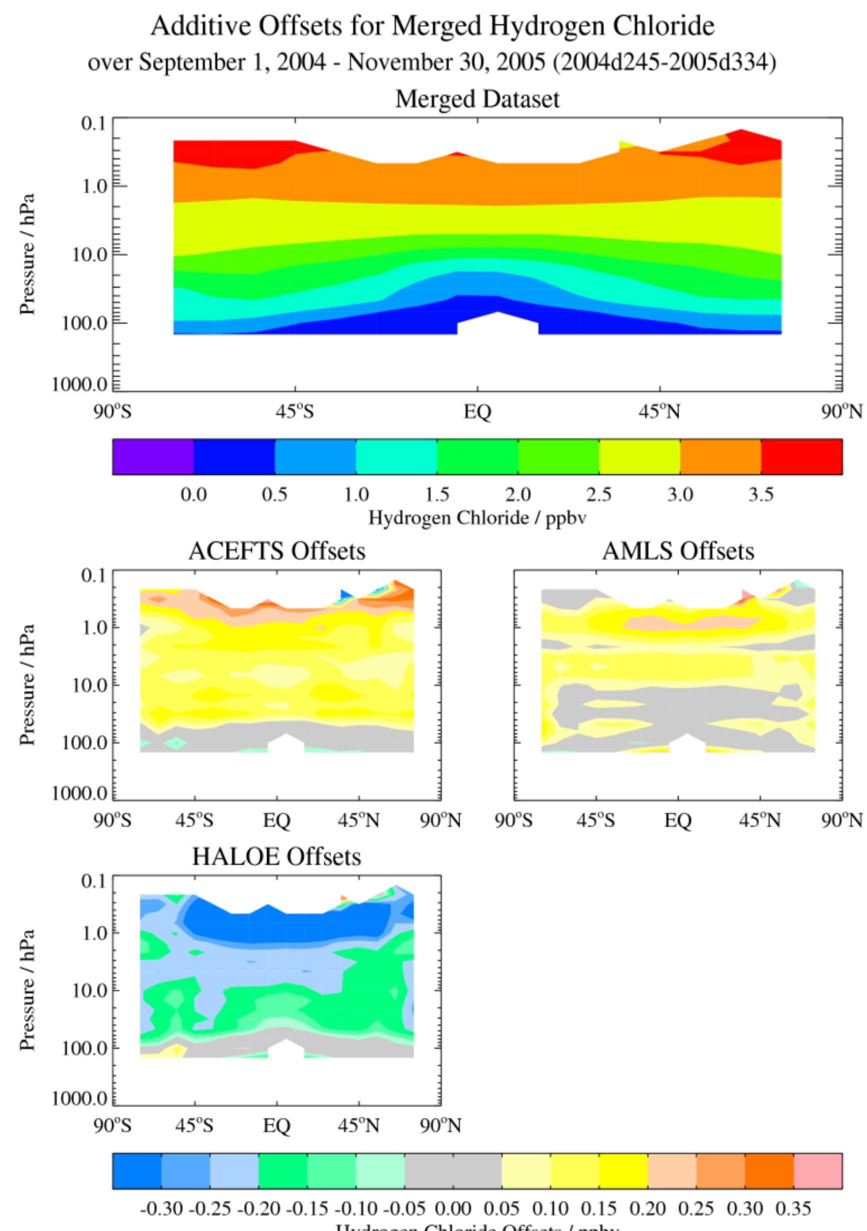
Illustration of poor monthly coverage overlap between stratospheric sounders [for some latitude ranges (tropics mainly)].



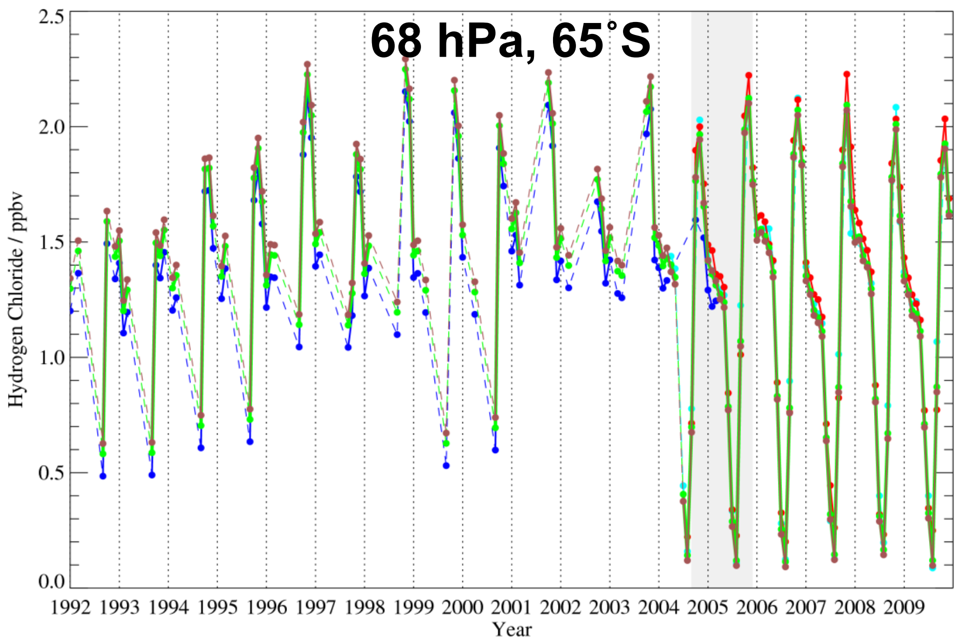
HCl: merging datasets, offset values

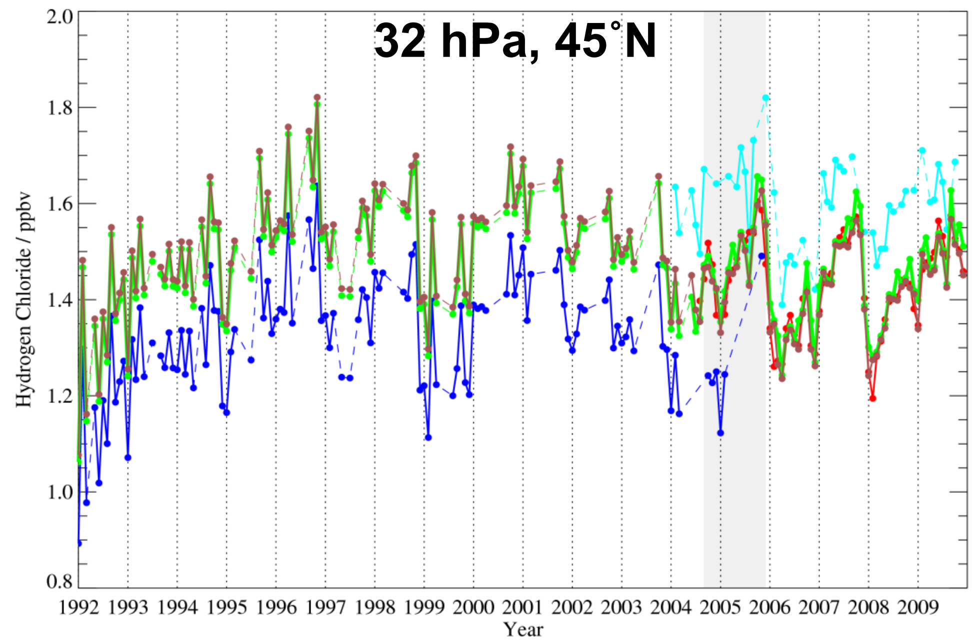
We go from no tropical overlap (left set of plots) with “direct” merge to “global” coverage / no gaps (right set of plots) with “iterative” merge





HCl Examples: HALOE, ACE-FTS, Aura MLS, Merged (direct), Merged (iterative)





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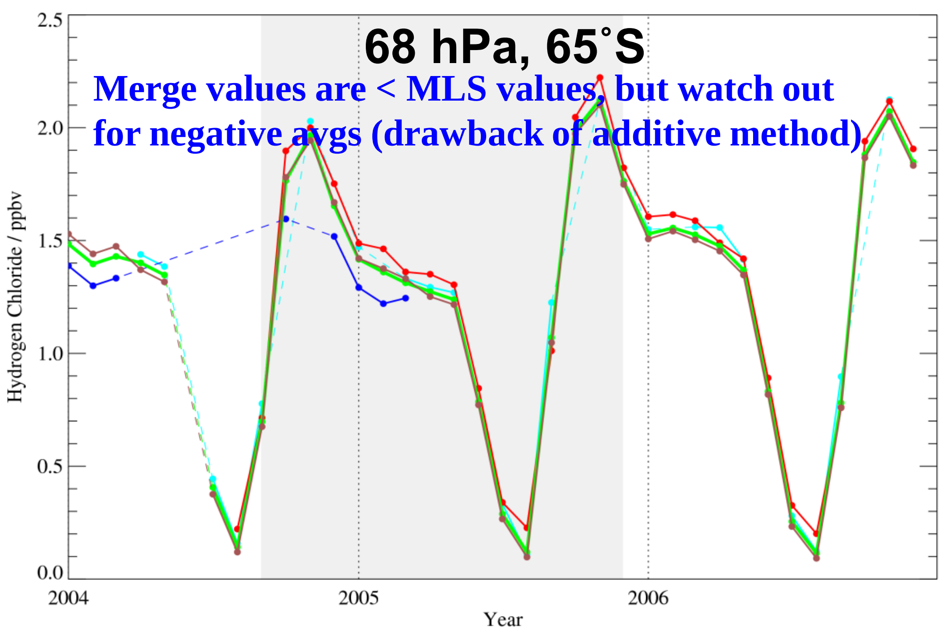
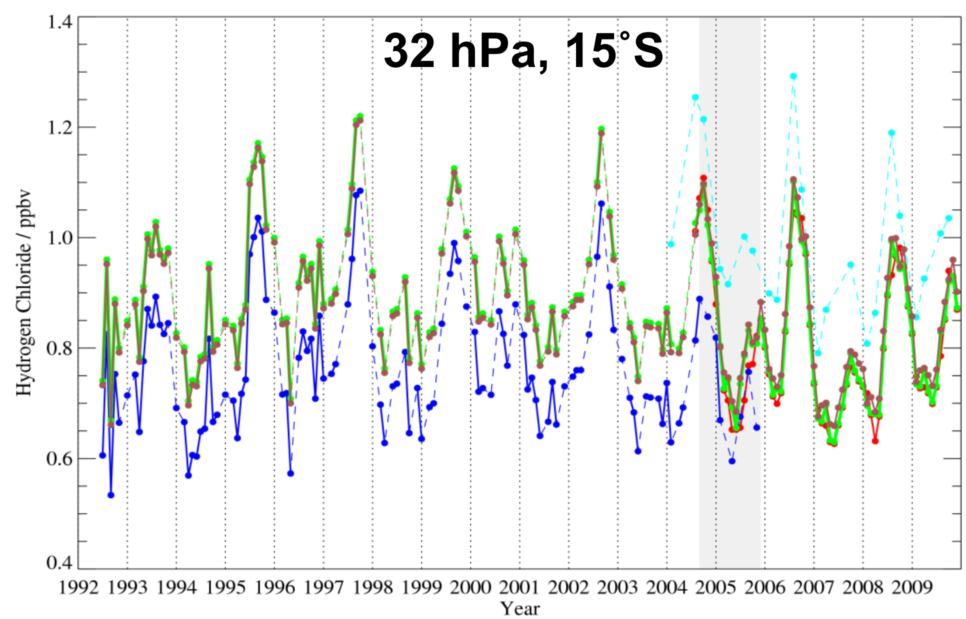
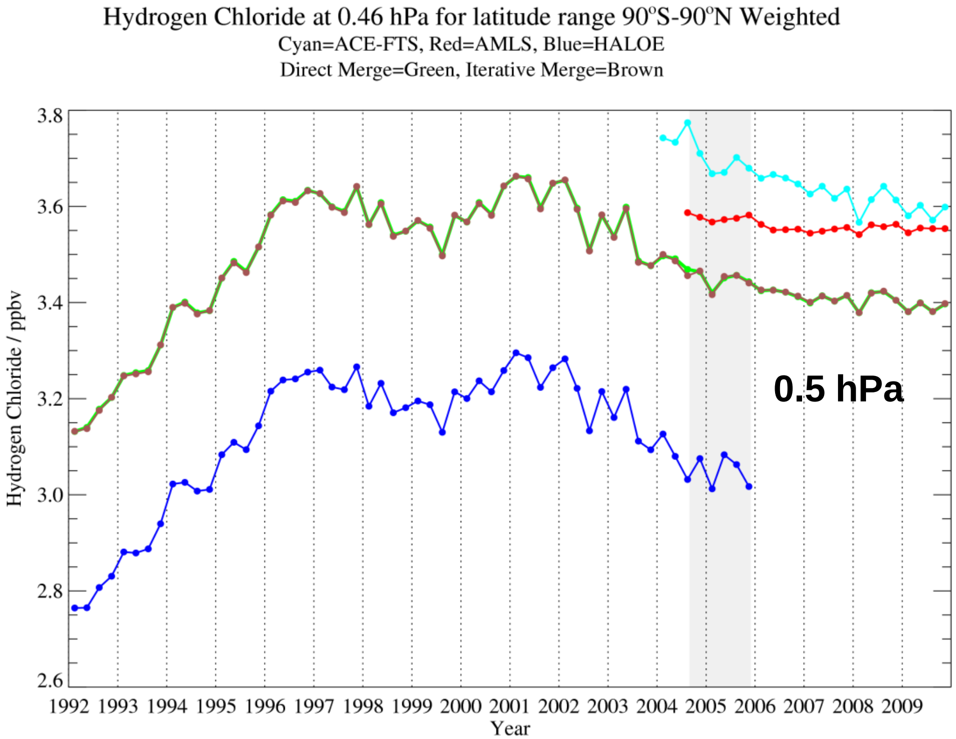
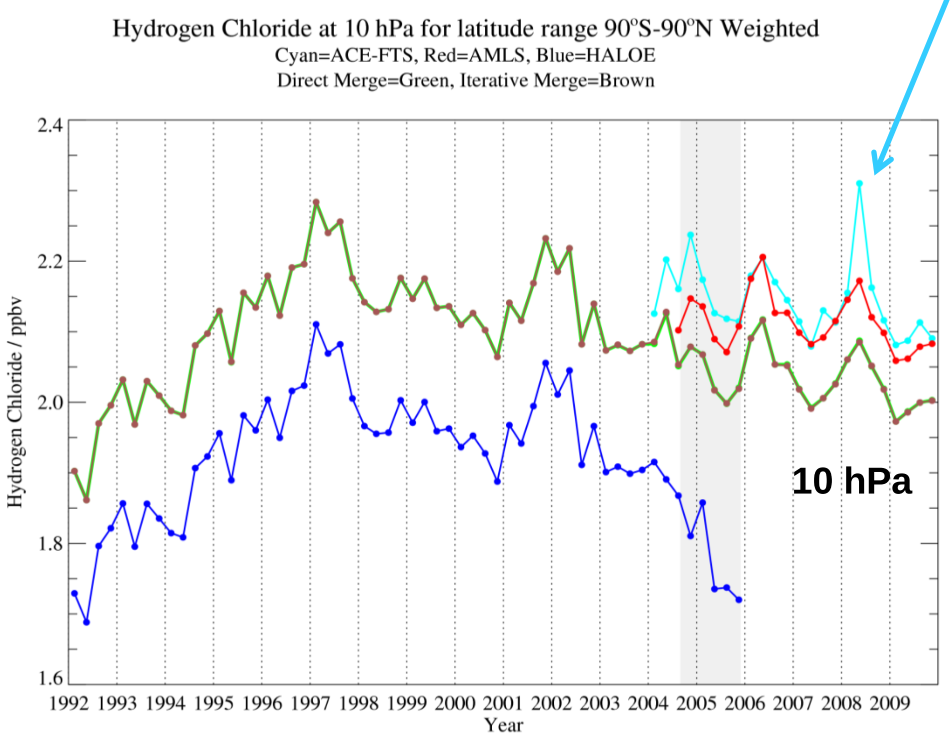








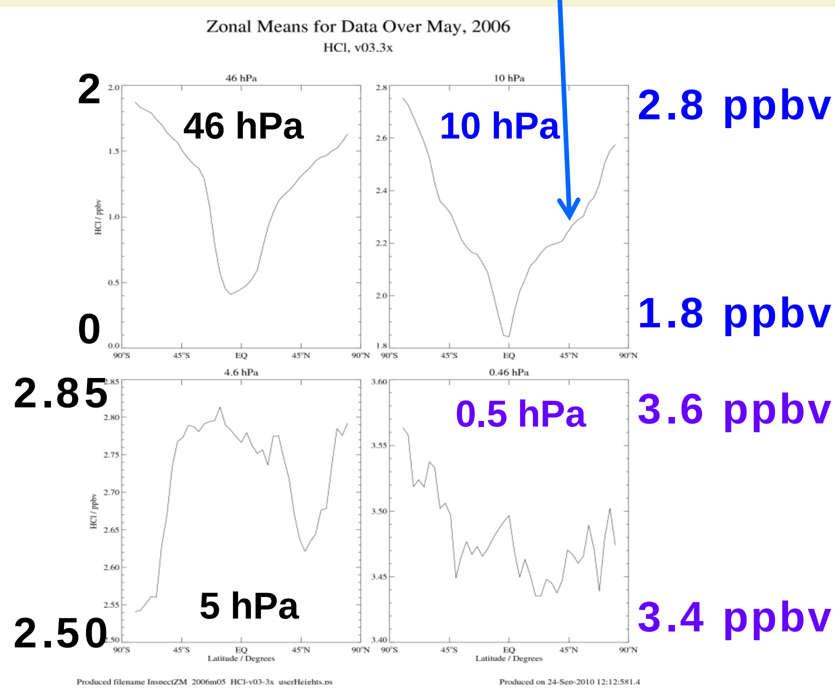
HCl: Seasonal and global averages

- Top panel: issues with upper stratospheric MLS trend
  → would bias a trend in merged product
- Bottom panel: 10 hPa values look more in line with ACE-FTS
  > also larger variability in LS (> 30%)

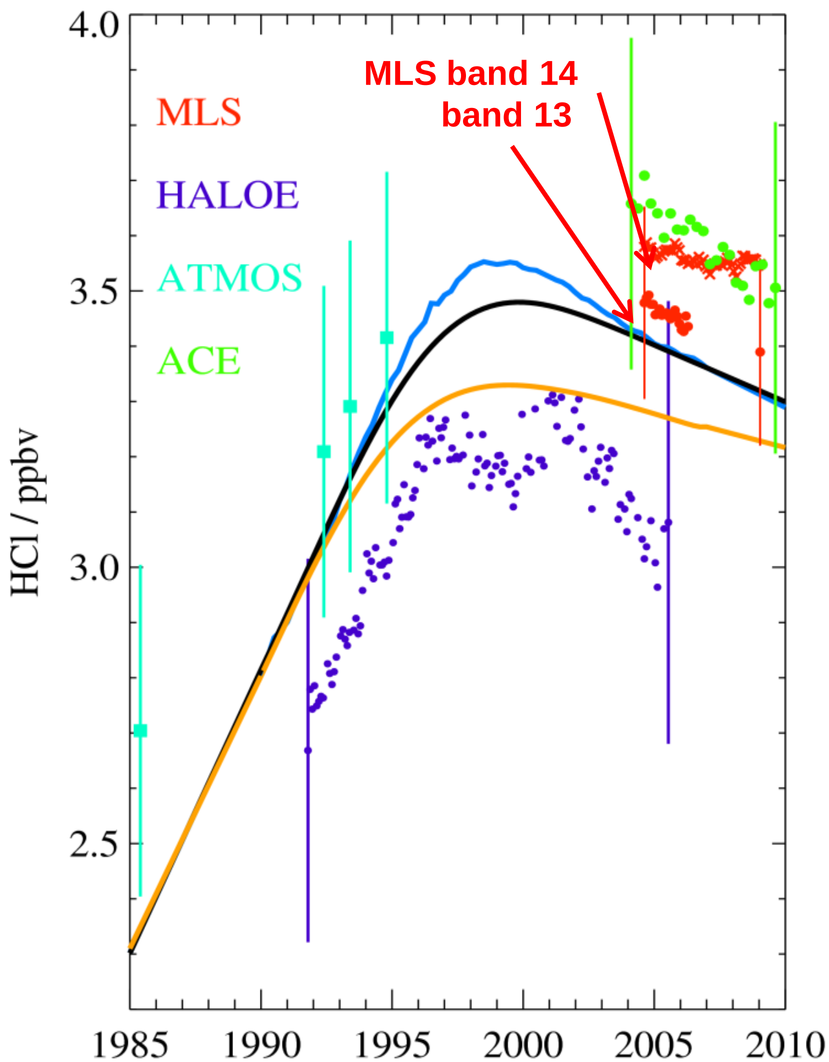
- However, there are also issues with representativeness **ACE-FTS global avgs.**

> even seasonal averages, especially if / as there are strong latitudinal gradients

> how best to restrict minimum number of profiles when doing "global" averages?



HCl: pressure range for MLS HCl



Overview of HCl trends (at ~ 55 km)
> datasets and expectations (curves)
[update to *Froidevaux et al*., 2006]

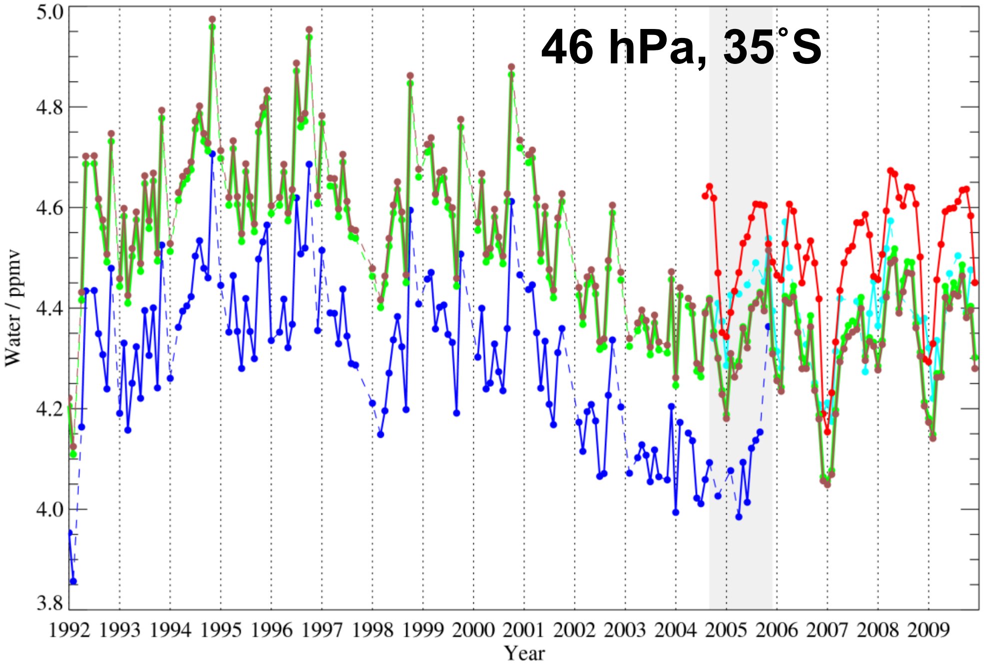
Unfortunately, there is a trend difference between the two MLS bands (for HCl data), certainly in the upper stratosphere

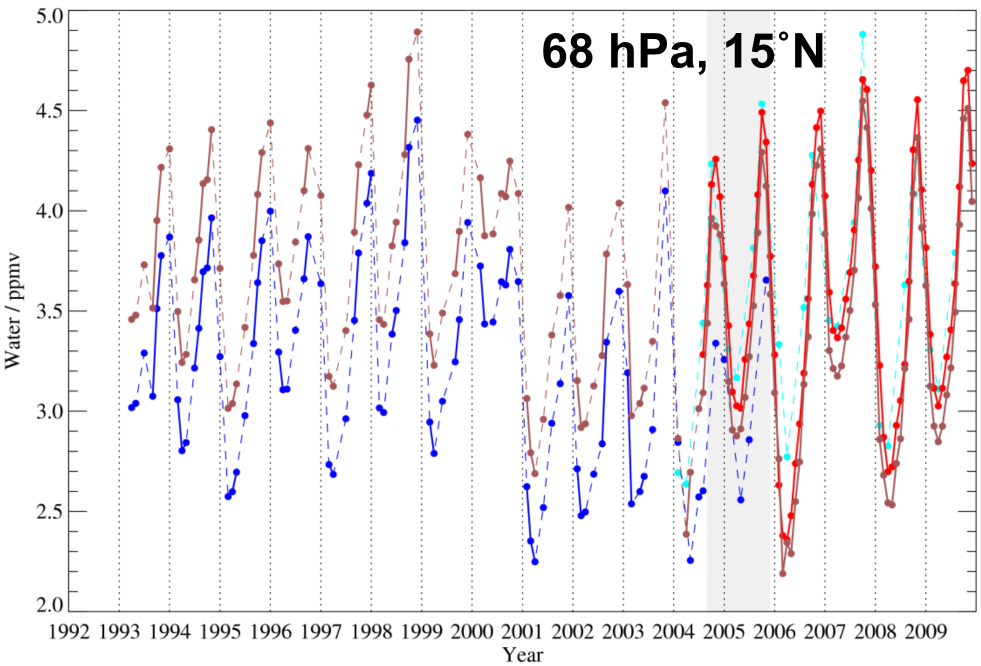
- band 13 targeted HCl initially, but now used sparingly (~3 days every 2 years), may fail within 1 to a few weeks of operation
- band 14 is used as a continuous backup, but shows too slow a trend in the upper stratosphere (vs ACE-FTS & expectations);

But for **lower stratosphere,**
B14 HCl data is OK (and useful) for merging
- larger variability in this region
(not as amenable to small HCl trend studies)
- HCl is not a total chlorine surrogate in LS

OR…maybe we create 2 merged HCl records
- one applicable to trends [with no MLS data]
- one for spatial/seasonal (and interannual) issues [with the MLS data/coverage]

H_2O Examples: HALOE, ACE-FTS, Aura MLS, Merged (direct), Merged (iterative)





The merging method is applied to H_2O, as another example with the same instruments performing the measurements [& no HCl-related MLS trend issue]

In general, sampling/coverage issues mean that fitting procedures should be applied (later) to the data record(s) if continuous time series are desired (e.g., more readily compared to models)
> although not needed for the more continuous sampling from emission instruments (like Aura MLS)

Ozone

- **O_3 datasets:** SAGE I, SAGE II, SAGE III, HALOE, UARS MLS, ACE-FTS, Aura MLS (+ POAM data mainly as a check)
  - Have performed checks of SAGE II dataset vs Randel and Wu (2007) ["raw" data]
    - Cross-check internally (data binning by R. Wang and J. Anderson)
      → looks like good agreement overall,
      but there is a small latitudinal shift [seems to be an issue with Randel/Wu data]

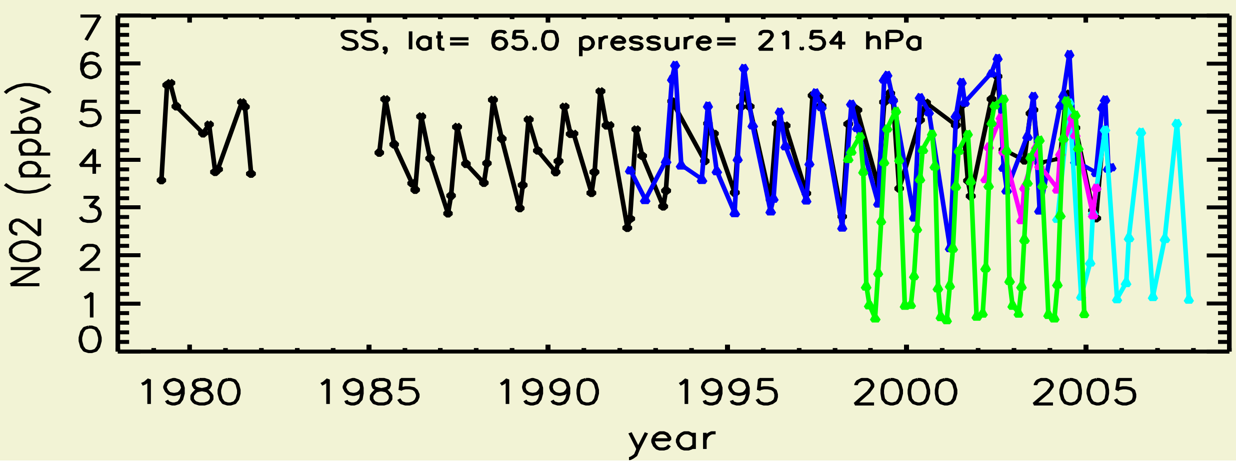
- **Merged ozone data (have added some refinements to merging procedure)**
  - Adjust and merge AMLS, UMLS, HALOE, and SAGE III using SAGE II as reference
  - Bring in ACE-FTS data versus this reference (check avg. offsets and adjust/merge) + special cases at the highest latitude bins [for continuity]

- **Ozone data in density (or DU) and altitude units [to come after VMR/p data]**
  - Need to interpolate MLS data from VMR/p grid to number density/z grid
  - HALOE, SAGE-II and ACE-FTS will also be used in density/z coordinates

- **Verification (validation) of data quality** [for merged data record]
  - Compare versus other long-term profiles
    > e.g., versus ground-based data
    > versus concurrent MEaSUREs work (McPeters et al. work on SBUV O_3 profiles)
    > versus other efforts (TBD)
    [if you wish to do intercomparisons, please contact us]
    - SPARC Data Initiative (Nov. meeting in Bern)
    - Also, Jan. 2011 meeting in UK (N. Harris et al.) on these topics (for O_3)
  - May also compare to column ozone from SBUV/TOMS/OMI

NO_2

- **Data:** **Use SAGE-II, HALOE, POAM-3, SAGE-III, and ACE-FTS NO_2 data**
- Need to group data based on *local* (SR/SS) *[+ better screening needed (for ACE-FTS)]*
- Need to work more on how to adjust for offsets
  - Larger differences between instruments compared to O_3
    - Also, HALOE applied a diurnal correction in retrieval, while other satellites did not have such correction [will play a role in offset values, but trends should be OK]
  - Recommendation: Use HALOE NO_2 (or HALOE/ACE-FTS avg.) as a reference
    - More latitudinal coverage (compared to POAM/SAGE-III)
    - SAGE-II (satellite) SR NO_2 data have low bias problem (thermal shock). By adjusting SAGE-II SR to HALOE, we can keep the SAGE-II SR record (extending the total time period and coverage).
  - Need to consider sampling issues when adjusting other data to HALOE
    - For local SS: seems to be OK (but needs further checking)
    - For local SR: no colocated (common) months for HALOE vs POAM-3 or SAGE-III, and no colocated months for HALOE/ACE-FTS (northern mid-to high lat.)
    - **Possible solutions**: extend offsets from other lats., use broader (seasonal averages) rather than monthly, or resort to fitting annual (+ maybe other) cycles for checking offsets



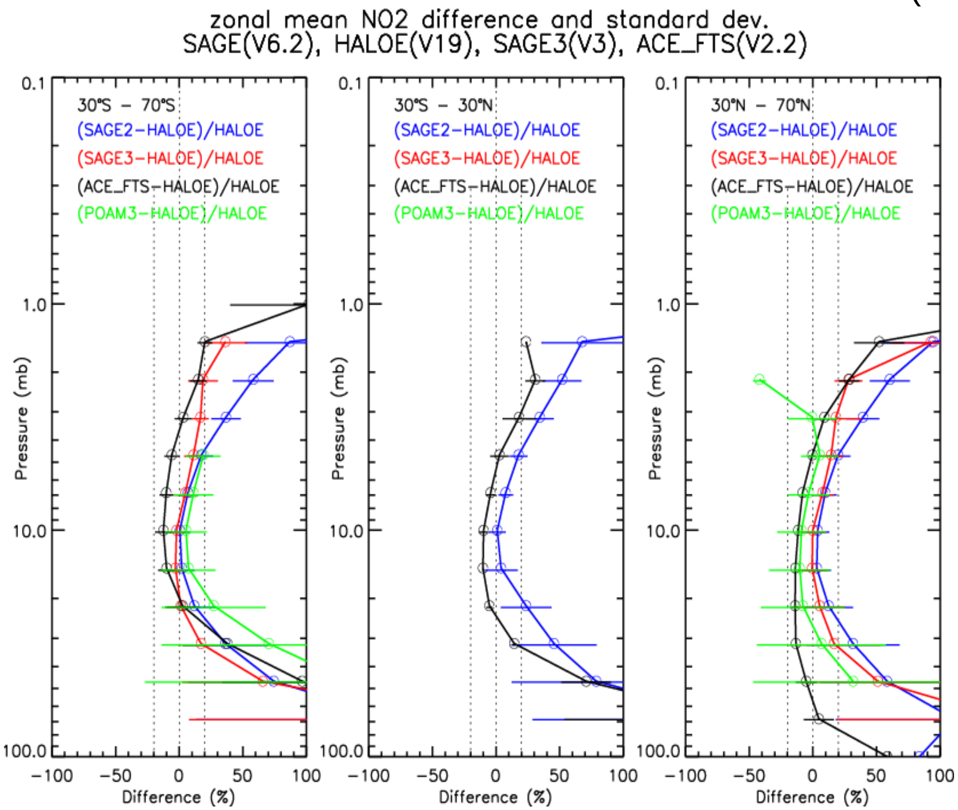
NO_2 (sunset):
SAGE-I/II, **HALOE**, **POAM-3**, **SAGE-III**, and **ACE-FTS** for 60°N-70°N at 22 hPa.

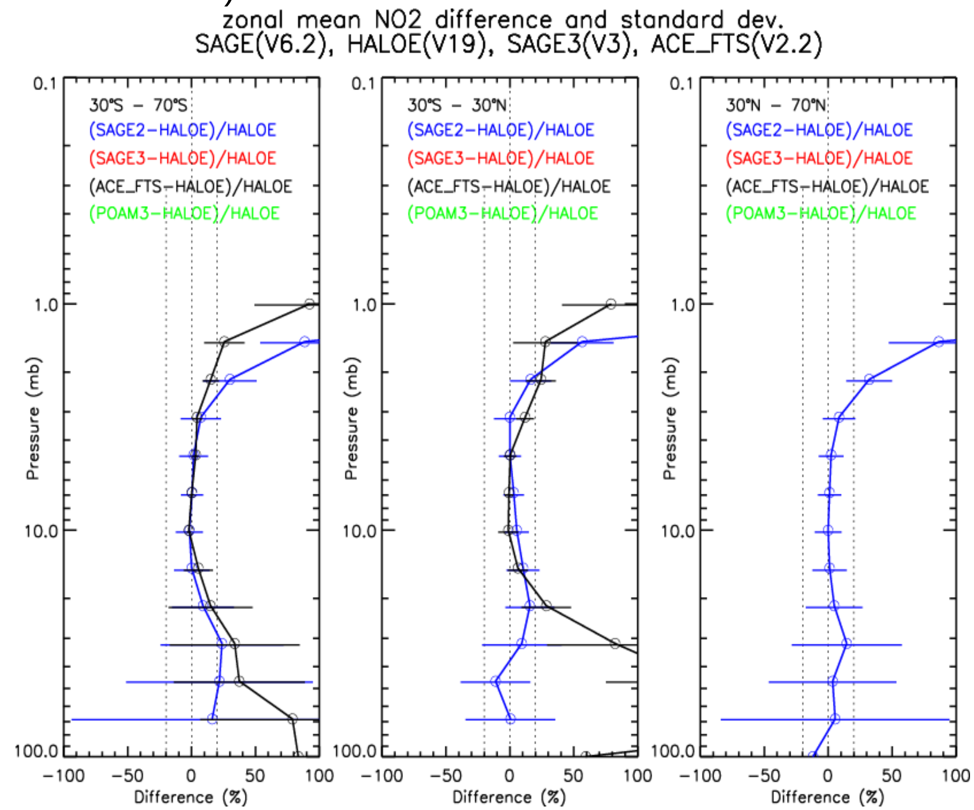
NO_2: Examples

NO_2 for local sunset

Comparisons are based on zonal means (not coincidences)

NO_2 for local sunrise



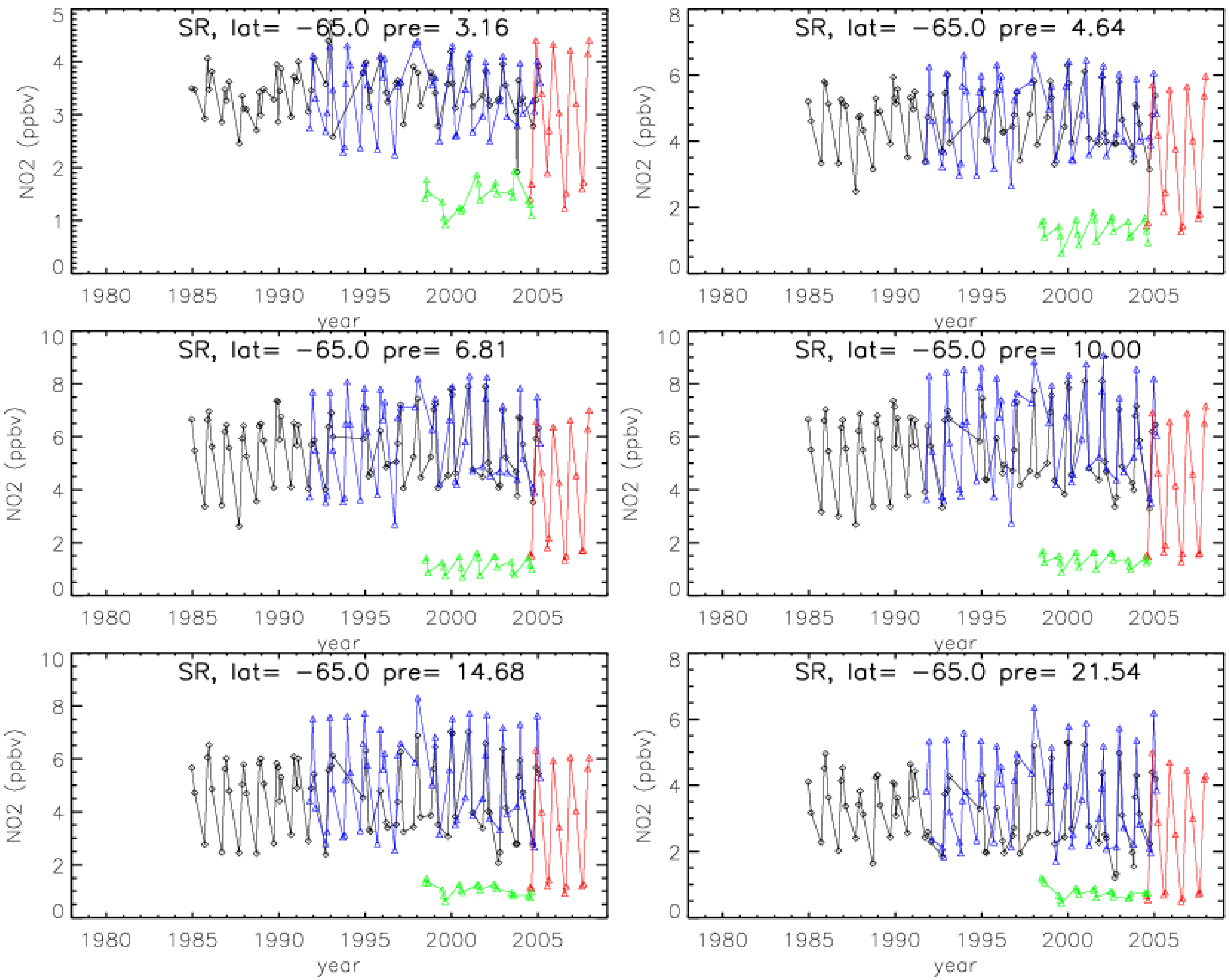


Sunset data: Based on these comparisons (and other reasons listed in previous slide), one should be able to adjust the sunset (SS) NO_2 instrument data with HALOE NO_2 used as a reference.

Sunrise data: these datasets have less common coverage between the 4 instruments - see also next slide.

NO_2: Examples

Time series of monthly zonal mean NO_2 during local sunrise



SAGE-II, HALOE, POAM-3, ACE-FTS

No colocated SR data between HALOE and POAM-3 in the S.H.

NO_2 varies seasonally and peaks in the summer

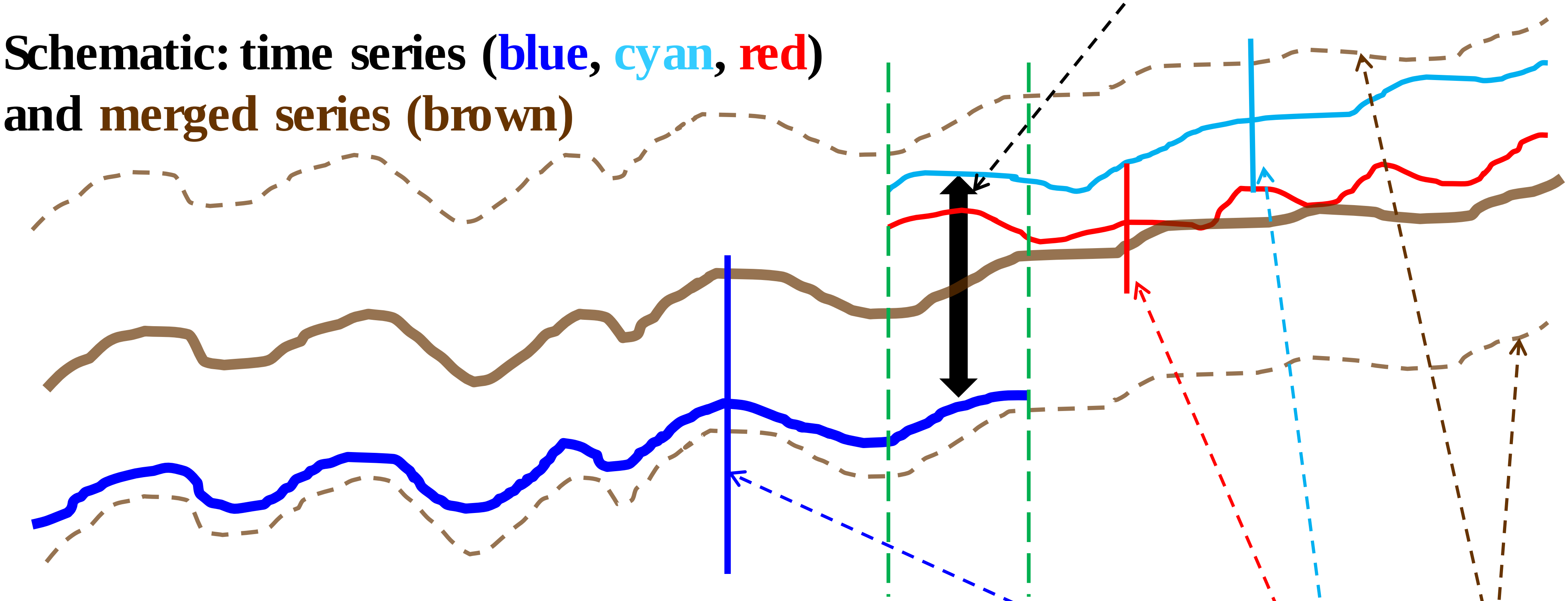
POAM-3 measured in Jun, Jul, Aug

while
HALOE & SAGE-II measured in
Oct to Mar

→ the POAM-3 sampling (SH winter months) is largely responsible for its apparent low bias

Other quantities of interest for data files: uncertainties, etc…

- Include information (for data users) regarding the average spread of measurements about the merged time series, within the overlap time period.
  > e.g., min, max departures and/or rms



- **Models can best be compared to merged data if estimated error bars (ranges) are provided with merged (and original individual) records.**
  > we will also (try to) compile error bar estimates (systematics) from each original source
  > also include std. deviations (about zonal means), number of profiles, sza information,…
- There is more than one way to provide such error bars… we will state/discuss what we provide.

Summary and further work

- **Merging of satellite datasets is proceeding for MEaSUREs GOZCARDS**
  > exploratory work is nearing an end

- **We now need to:**
- Finalize file contents/formats
- Improve data screening (e.g., outliers from the ACE-FTS datasets)
- Finalize latitude and pressure ranges, and consider special cases (merging procedure, consistency issues) at high latitudes in particular
- Consider including new data versions
  > e.g., use MLS v3.3 instead of or after the v2.2 data? (TBD, pros & cons)
- Double-check the work, look through many plots, etc… for robustness

- **Cross-calibration work versus ground-based datasets** is another useful aspect, especially to help tie satellite datasets across large data gaps (e.g., for UARS and Aura MLS cross-calibration - ClO, HNO_3)

- **Ambitious (5-yr) project with many species/products**
  > scheduled for many data record deliveries this coming year and public access: JPL GOZCARDS website and via GES DISC
  > will look for other intercomparison opportunities – and early user feedback…

- **Contact us if interested and/or with comments!** **(Lucien.Froidevaux@jpl.nasa.gov)**